A Novel Numerical Scheme for Nonhomogeneous Diffusion Processes in Irregular Domain

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ABSTRACT

In this paper, a novel numerical scheme (FDMFS), which combines the finite difference method (FDM) and the method of fundamental solutions (MFS), is proposed to simulate the nonhomogeneous diffusion problem. Although the time-dependent MFS is meshless, extendable for any dimensional problems and without transformation or difference discretization for the time domain, the MFS is only useful for dealing with homogeneous partial differential equations. Therefore, we proposed the FDM with Cartesian grid to handle the non-homogeneous term of the equations. The numerical solution in FDMFS is decomposed as a particular solution and a homogeneous solution. The particular solutions are constructed using the FDM in an artificial regular domain which contains the real domain, and the homogeneous solutions can be obtained by the time-space unification MFS. Besides, the Cartesian grid for particular solution is very simple to generate automatically. We proposed three different treatments for particular solution and compared these schemes with each other. Two numerical examples are chosen to validate the proposed numerical scheme and the numerical results are compared well with analytical solutions

Keywords: non-homogeneous, diffusion, finite difference method, method of fundamental solutions, irregular domain.

1. INTRODUCTION

Many physical problems, such as heat transfer, pollution transports, chemical processes etc, are usually governed by diffusion equations. Some external input of energy is represented in the form of a forcing function by the nonhomogeneous term. Classical numerical methods, such as FDM, finite element method (FEM), finite volume method (FVM), had adopted to simulate the diffusion equations. However, all of they are mesh-dependent method and need mesh generation. Especially for irregular domain, the FDM needs the complicated transformations of coordinate. The associated bookkeeping of the elements and nodes is also cumbersome and expensive in the CPU time. Recently, a lot of attractive meshless or meshfree methods are developed and applied to solve diffusion equations.

Meshless numerical method is clever at the problems in irregular domain. As the name implies, the meshless method is a kind of numerical scheme without mesh but require only nodes for boundary and initial conditions. There are a lot of researches on meshless methods for diffusion problems, such as radial basis function (RBF) collocation method or Kansa method [1], indirect radial basis function network (IRBFN) method [2], meshless local Petrov-Galerkin (MLPG) method [3], and the MFS [4-5].

In this research, we applied the MFS based on time-dependent fundamental solutions. The MFS is also known as F-Treffz method or singularity method and was presented firstly by Kupradze and Aleksidze [6] in 1964. The MFS is applied widely to simulate physical problems, for example the Helmholtz equation [7-9], potential problem [10], Stokes flow [11-13] and diffusion problem [14-15]. In another words, the MFS is good at solving homogeneous partial differential equations (PDEs). In order to extend the MFS to solve nonhomogeneous PDEs, we have to combine MFS with other numerical scheme.

When the PDEs have steady forcing functions, Burgess and Mahaherin [16] constructed the particular solutions by direct numerical domain integration. In 1995, Chen [17] employed the quasi-Monte Carlo (QMC) quadrature as numerical integration to find the particular solutions. Golberg [18] suggested the MFS to solve Poisson's equation by approximating the forcing function by thin plate splines (TPSs). Henceforward, the MFS is extended for nonhomogeneous partial differential equations by combining the dual reciprocity method (DRM) where the forcing function is approximated by a finite series of radial basis functions (RBFs) [19-21].

Golberg and Chen [22] used the MFS based on modified Helmholtz fundamental solution to simulate the nonhomogeneous diffusion equations via associating with the DRM in 1998. Chebyshev interpolation [23] is also suggested to approximate the right-hand side of Helmholtz-type equations for diffusion problems. On the other hand, Young's group concentrates on developing another scheme which uses the time-space unification diffusion fundamental solutions [4]. Young, Tasi and Fan

[14] extended the time-dependent diffusion DRM-MFS (or MPSMFS) model to solve multidimensional nonhomogeneous diffusion problem and they also give a comparison between their proposed scheme and Golberg and Chen's research [22]. Two years later, Young, Chen, Fan and Tsai [24] combined the MFS and eigenfunction expansion method (EEM) to simulate the same equation. Unfortunately, all of these methods can not be applied directly for diffusion problems with time-dependent forcing function.

This research proposes a numerical scheme to extent the MFS for diffusion equation with unsteady forcing function. The solution of a nonhomogeneous PDE can be split into the summation of particular solution and homogeneous solution. We use the FDM to solve the particular solution in an artificial orthogonal grid which contains the physical domain and the time-dependent MFS to solve the homogeneous diffusion solutions. The concept is similar to the research of Chantasiriwan [25] who combined the FDM and MFS to solve the steady Poisson problem.

The aim of this study is to demonstrate the capability of the proposed FDMFS for diffusion equation with unsteady forcing function. The governing equations and numerical method will be explained in sections 2 and 3, individually. The numerical results and conclusions will be provided in sections 4 and 5. There are two problems adopted in the paper and the results are compared well with the analytical solutions.

2. GOVERNING EQUATIONS

The diffusion equation with unsteady forcing function over the problem domain Ω with boundary Γ can be written as follows:

$$\frac{\partial T(\vec{x},t)}{\partial t} = k\nabla^2 T(\vec{x},t) + F(\vec{x},t) \tag{1}$$

where $\vec{x}$ is the general spatial coordinate, t is the time, k is the diffusion coefficient, $F(\vec{x},t)$ is the forcing function, and $T(\vec{x},t)$ is the scalar variable to be determined. The initial condition of the problem is

$$T(\vec{x},t_0) = f_1(\vec{x}) \text{ in } \Omega \tag{2}$$

with the Dirichlet and Neumann boundary conditions.

$$T(\vec{x},t) = f_2(\vec{x},t) \text{ in } \Gamma_1 \tag{3}$$

$$\frac{\partial}{\partial n} T(\vec{x},t) = f_3(\vec{x},t) \text{ in } \Gamma_2 \tag{4}$$

where Ω is the problem domain, $\Gamma_1+\Gamma_2$ is equal to the boundary Γ, n is the normal direction and $f_1(\vec{x})$, $f_2(\vec{x},t)$, $f_3(\vec{x},t)$ are known functions.

3. NUMERICAL METHOD

3.1 Basic Numerical Scheme

The solution $T(\vec{x},t)$ can be written as the linear combination of homogeneous solution $T_h(\vec{x},t)$ and particular solution $T_p(\vec{x},t)$ shown as follows:

$$T(\vec{x},t) = T_h(\vec{x},t) + T_p(\vec{x},t) \tag{5}$$

The nonhomogeneous equation governs the particular solution shown as follows:

$$\frac{\partial T_p(\vec{x},t)}{\partial t} - k\nabla^2 T_p(\vec{x},t) = F(\vec{x},t) \tag{6}$$

No boundary condition is needed and the initial condition can be set as an arbitrary function; the homogeneous equation governs the homogeneous solutions.

$$\frac{\partial T_h(\vec{x},t)}{\partial t} - k\nabla^2 T_h(\vec{x},t) = 0 \tag{7}$$

with the modified initial condition

$$T_h(\vec{x},t_0) = f_1(\vec{x}) - T_p(\vec{x},t_0) \text{ in } \Omega \tag{8}$$

and the modified Dirichlet and Neumann boundary conditions

$$T_h(\vec{x},t) = f_2(\vec{x},t) - T_p(\vec{x},t) \text{ in } \Gamma_1 \tag{9}$$

$$\frac{\partial}{\partial n} T_h(\vec{x},t) = f_3(\vec{x},t) - \frac{\partial}{\partial n} T_p(\vec{x},t) \text{ in } \Gamma_2 \tag{10}$$

The numerical procedure starts from the particular solution. First of all, as shown in Fig. 1 (a)-(b), we need to distribute an orthogonal mesh which has to embed in the problem domain.

Next, we can use the FDM to simulate the particular solution by Eq.(6). As the fully explicit central difference scheme,

$$\begin{aligned} T_p^{n+1}(\vec{x},t) &= T_p^n(\vec{x},t) \\ &+ \Delta t \left\{ k \left[\frac{T^n_{p,i+1,j}(\vec{x},t) - 2T^n_{p,i,j}(\vec{x},t) + T^n_{p,i-1,j}(\vec{x},t)}{(\Delta x)^2} \right] \right\} \\ &+ \Delta t \left\{ k \left[\frac{T^n_{p,i,j+1}(\vec{x},t) - 2T^n_{p,i,j}(\vec{x},t) + T^n_{p,i,j-1}(\vec{x},t)}{(\Delta y)^2} \right] \right\} \\ &+ \Delta t \left[F^n(\vec{x},t) \right] \end{aligned} \tag{11}$$

where $\Delta t = \Delta t_p$ is the time step size for particular solution, Δx is the mesh size in x direction and Δy is the mesh size in y direction. Indeed, the implicit finite difference scheme also can be adopted to obtain the particular solution

$$T_p^{n+1}(\vec{x},t) - \Delta t\left\{k\left(\frac{T_{p,i+1,j}^{n+1}(\vec{x},t) - 2T_{p,i,j}^{n+1}(\vec{x},t) + T_{p,i-1,j}^{n+1}(\vec{x},t)}{(\Delta x)^2}\right)\right\} - \Delta t\left\{k\left(\frac{T_{p,i,j+1}^{n+1}(\vec{x},t) - 2T_{p,i,j}^{n+1}(\vec{x},t) + T_{p,i,j-1}^{n+1}(\vec{x},t)}{(\Delta y)^2}\right)\right\} = T_p^n(\vec{x},t) + \Delta t\left[F^n(\vec{x},t)\right] \tag{12}$$

The initial condition of the particular solution can be assumed as an arbitrary function and the boundary condition of the particular solution is not required. By the advantage of explicit FDM, the particular solution can be obtained in a very short time and no matrix solver is needed.

After the particular solution is obtained, the meshless MFS is considered to solve the homogenous solution. The homogeneous solution satisfies the linear diffusion equations, Eq. (7), and the modified initial and boundary conditions, Eq. (8)-(10). In MFS, the diffusion solution can be represented as the linear combination of the diffusion fundamental solutions with different intensities. The fundamental solution of the linear diffusion equation is governed by

$$\frac{\partial G\left(\vec{x},t;\vec{\xi},\tau\right)}{\partial t} = k\nabla^2 G\left(\vec{x},t;\vec{\xi},\tau\right) + \delta\left(\vec{x}-\vec{\xi}\right)\delta\left(t-\tau\right) \tag{13}$$

where $G\left(\vec{x},t;\vec{\xi},\tau\right)$ is the fundamental solution of the diffusion equation. $\vec{x}=(x,y)$ and $\vec{\xi}=(\xi,\eta)$ are the spatial coordinates of the field point and source point, as t and τ are the temporal coordinates of the field point and source point. $\delta(\ )$ is the well-known Dirac delta function.

By taking the Fourier transform and the inverse Fourier transform of the above equation, the free-space Green's function or the fundamental solution of the diffusion equation can be obtained as:

$$G\left(\vec{x},t;\vec{\xi},\tau\right) = \frac{e^{-\frac{\left|\vec{x}-\vec{\xi}\right|^2}{4k(t-\tau)}}}{\left(4\pi k\left(t-\tau\right)\right)^{d/2}} H\left(t-\tau\right) \tag{14}$$

where d is the number of spatial dimension and equal to two in this study. $H(\ )$ is the Heaviside step function.

Based on the time-dependent MFS, the homogeneous solution can be expressed as the linear combination of the diffusion fundamental solutions

$$T_h\left(\vec{x},t\right) = \sum_{j=1}^{N_h} \alpha_j G\left(\vec{x},t;\vec{\xi}_j,\tau_j\right) \tag{15}$$

where N_h is the number of source point. In our numerical experiments, the numbers of field points and source points are chosen as the same, $N = N_h$. α_j is the unknown coefficient which denotes the intensities of the corresponding fundamental solutions.

The initial and boundary conditions of homogeneous solution are modified by the particular solution:

$$T_h(\vec{x},t_0) = T(\vec{x},t_0) - T_p(\vec{x},t_0) = f_1\left(\vec{x}\right) - T_p(\vec{x},t_0) \text{ in } \Omega \tag{16}$$

$$T_h(\vec{x},t) = T(\vec{x},t) - T_p(\vec{x},t) = f_2\left(\vec{x},t\right) - T_p(\vec{x},t) \text{ in } \Gamma_1 \tag{17}$$

$$\frac{\partial}{\partial n}T_h(\vec{x},t) = \frac{\partial}{\partial n}T(\vec{x},t) - \frac{\partial}{\partial n}T_p(\vec{x},t) = f_3\left(\vec{x},t\right) - \frac{\partial}{\partial n}T_p(\vec{x},t) \text{ in } \Gamma_2 \tag{18}$$

Applying the concept of the MFS, a matrix form is obtained as follows:

$$\begin{bmatrix} G\left(\vec{x},t_0;\vec{\xi}_j,\tau_j\right) \\ G\left(\vec{x},t;\vec{\xi}_j,\tau_j\right) \\ \frac{\partial}{\partial n}G\left(\vec{x},t;\vec{\xi}_j,\tau_j\right) \end{bmatrix}\left\{\alpha_j\right\} = \begin{Bmatrix} f_1(\vec{x},t_0) \\ f_2(\vec{x},t) \\ f_3(\vec{x},t) \end{Bmatrix} \tag{19}$$

Solving the above matrix, the coefficients α_j are obtained, and then the homogeneous solutions can be acquired by Eq. (15). Lastly, the numerical solutions can be obtained by summing up the particular and homogeneous solutions, Eq. (5).

As shown in Fig. 1 (c), the meshless MFS requires only field points for boundary and initial conditions without mesh. The locations of field and source points of MFS are illustrated as Fig. 2. The field and source points are located at the same spatial positions but different time levels. The parameter, λ, shown in Fig. 2 is chosen as $\lambda = 0.5R/k$ in this study and R is the maximum length in the domain of the problem.

Although, the time increment of FDM scheme, Δt_p, should satisfied the stability condition, the homogeneous solution doesn't need to be solved at each time step. In other words, the time interval for the MFS can use a large one. In this paper, we adopt $\Delta t_h = 10\Delta t_p$ or $\Delta t_h = 100\Delta t_p$. Therefore, the CPU time of the simulation can be shortened. In order to demonstrate the idea of FDMFS more simply and

clearly, the illustration of numerical procedure is shown as Fig. 3.

3.2 Manipulation in irregular domain

The present numerical scheme can solve problems with irregular domain directly. For solving particular solutions by FDM, we set a simple uniform Cartesian mesh, Ω^C, which covers the whole real problem domain Ω as a computational domain for particular solution. The Cartesian mesh Ω^C can be divided into two parts. One is the interior of the problem Ω_i^C domain Ω. The other one is exterior of the problem Ω_e^C domain Ω.The particular solution at each point is governed by Eq. (6). However, we have a trouble that the unknown forcing function on Ω_e^C is unknown in most practical problems. Therefore, we proposed three different schemes illustrated as Fig. 4 to overcome this issue. The accuracy and efficiency of these methods are compared with each other in section 4.

3.2.1 Method 1(M1)

Provided that the forcing function of the problem is spatial-independent or the forcing function on exterior Ω_e^C of the problem domain is known, the governing equation, Eq (6), can be applied doubtless. In other words, we use the same FDM to discretize the nonhomogeneous diffusion equation to obtain the particular solution on both Ω_e^C and Ω_i^C. The FDM scheme is the same as the FDM for a nonhomogeneous diffusion problem with a rectangular domain.

The idea of this method is simple and no extra computer code is required. This method has high accuracy due to no unreasonable assumptions. The virtual Cartesian mesh for particular solution can be constructed automatically by known maximum and minimum value on each coordinate. This work won't affect the efficiency of the numerical scheme. However, this method is only suitable for the case which the forcing function is spatial-independent or the forcing function on the exterior Ω_e^C of the problem domain is known. Otherwise, we need to consider M2 or M3.

3.2.2 Method 2(M2)

We can assume that this forcing function exterior the problem domain is equal to a constant, zero or a known physical value on the boundary. Therefore, the forcing function will appear a discontinuity near the boundary. Due to the nature of the FDM, the discontinuity will produce errors near the boundary and pollute the numerical results. Hence, we interpolate the forcing functions on the exterior domain Ω_e^C in order to smooth the forcing function on the Cartesian mesh Ω^C. If the forcing function on the computational domain for particular solution Ω^C is discontinuous, numerical error would be produced. To put it simply, the basic idea of M2 is to create a smooth forcing function to make the numerical scheme for particular solution can be applied successfully.

In most practical problem, the problem domain is usually irregular and the forcing function outside the problem domain Ω is unknown definitely. The M2 is developed to deal with this kind of problems. The unknown forcing function on the exterior domain Ω_e^C is set as a constant. The constant value can be defined through the system program and interpolations can be adopted to smooth the forcing function. This work needs to add computer code and set a rule to avoid discontinuous forcing function on the computational domain Ω^C for the particular solution. The scheme would increase the CPU time of the simulation. However, this one conforms to the practice problem mostly.

3.2.3 Method 3(M3)

In M3, we divide the numerical scheme into two parts. One is for nodes on the interior domain Ω_i^C. The particular solution is obtained by the original governing equation, Eq. (6). The other one is for nodes on the exterior domain Ω_e^C. The particular solution is equal to previous step without calculating. We don't care the particular solution on the non-real domain Ω_e^C in this method. However, some numerical error is caused by the inaccurate particular solution on the boundary.

This method can speed up the numerical scheme due to no calculating the particular solution on the non-real domain Ω_e^C.

.After the brief introduction of the three methods, we can expect that the M1 has high accuracy; M2 is the most useful one; M3 can obtain the rough numerical results in a short time. The detailed comparison of these three methods will be performed in the following section.

4.NUMERICAL EXPERIMENTS and RESULTSN

To illustrate the advantages of the proposed meshless scheme, there are two cases tested with irregular domains. Case 1 demonstrates the application of FDMFS for circular domains. A twin circle domain problem is adopted in case 2.

Case 1

We consider the forcing function is dependent on *x*, *y*, and *t*. The analytical solution is shown as follows:

$$T(\vec{x},t)=\left(\mathrm{Sin}(\pi x)+\mathrm{Sin}(\pi y)\right)\mathrm{Exp}\left(-k\pi^2 t\right) + (1+x)(1-x)(1+y)(1-y)\mathrm{Sin}(2\pi t)+10 \quad (20)$$

and the forcing function is

$$F(\vec{x},t) = 2\pi\left(x^2-1\right)\left(y^2-1\right)\mathrm{Cos}\ (2\pi\ t) \\ -2k\left(x^2+y^2-2\right)\ \mathrm{Sin}\left(2\pi\ t\right) \quad (21)$$

The forcing function is dependent on x, y and t. Fig. 5 (a) plots the time history of numerical results at (x,y)=(0.5,0.5) by M1, M2 and M3 and shows good agreement with analytical solutions. Fig. 5(b) shows that the maximum relative errors of M1, M2 and M3 are all less than 0.1%. The contour maps are shown in Fig. 6 for k=1 at t=0.1 ant t=0.25.These three methods for handling the irregular domain can produce reasonable results for arbitrary domain problem.

Case 2

The second case is considered to simulate problem with a twin circle domain. The analytical solution is chosen the same as case 1 and k=1. The maximum relative error is depicted in Fig. 7 and all of them are less than 0.1%. Moreover, Fig. 8 shows the contour maps via M1, M2 and M3 when t=0.10 and t=0.25. From this figure, we find the M3 has some error due to the discontinuity of the forcing function near the boundary.

5. CONCLUSIONS

The proposed FDMFS which is the combination of the conventional FDM and the meshless MFS is used to solve the diffusion equation with unsteady forcing function. The solutions are assumed as the combination of particular solutions and homogeneous solutions. The particular solutions are solved by the conventional FDM with a simple Cartesian grid which covers the whole physical domain. On the other hand, the homogeneous solution which is governed by the linear diffusion equation is solved by time-dependent MFS. Finally, the numerical solutions are obtained by summing the particular solutions and homogeneous solutions. The present numerical scheme can solve the diffusion equation with a time-dependent forcing function successfully. In addition, the boundary conditions for particular solution are needless and the initial conditions for particular solution can be assumed as an arbitrary function in the present scheme.

6. ACKNOWLEDGEMENT

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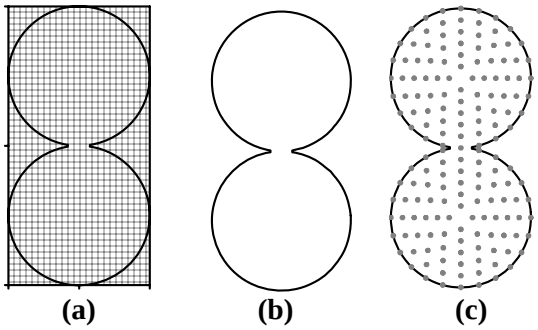
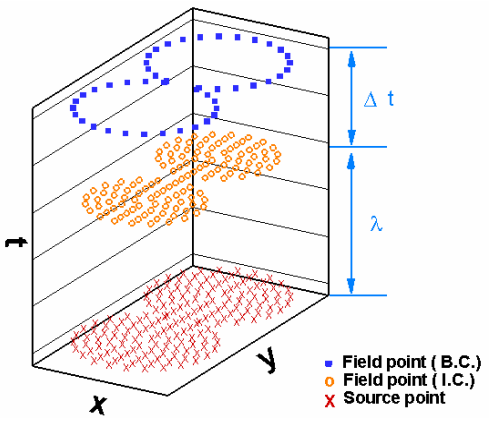
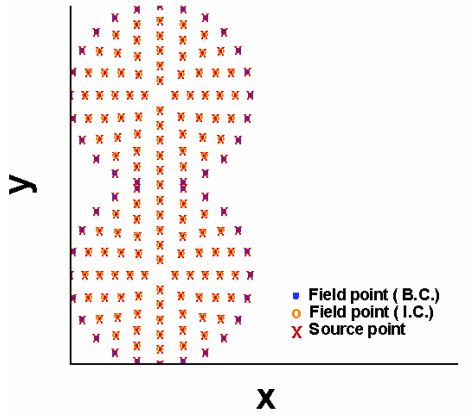


Figure 1: (a) FDM mesh (b) Problem domain (c) Node distribution of MFS



(a)



(b)

Figure 2: Schematic diagram of source and field points for the MFS based on diffusion fundamental solution (a) in a time-space coordinate (b) in a space coordinate

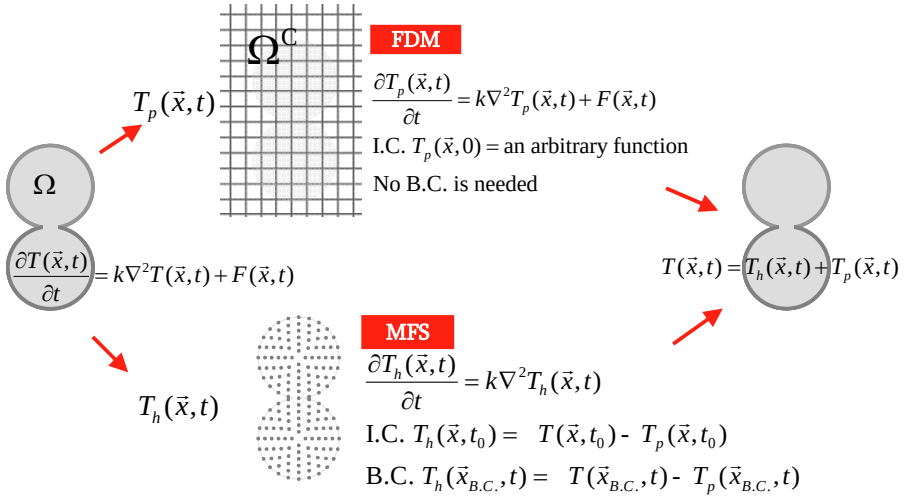


Figure 3: The illustration of the proposed numerical scheme (FDMFS)

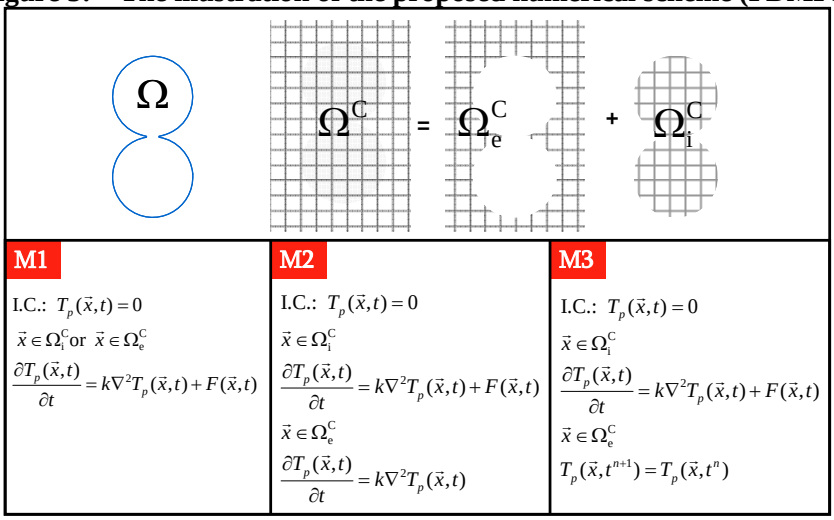
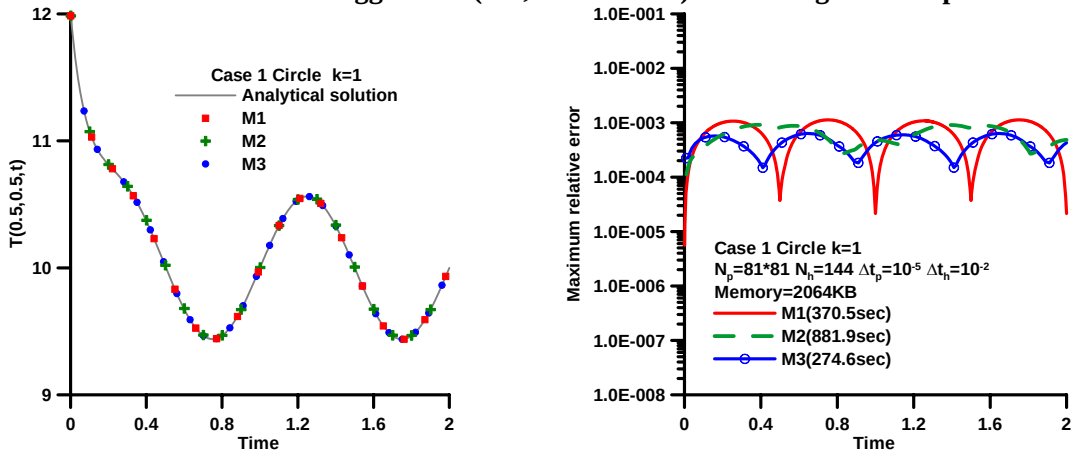


Figure 4: The illustration of three suggestions (M1, M2 and M3) for dealing with the particular solutions.



(a) (b)

Figure 5: Time history of (a) temperature at (0.5, 0.5) and (b) maximum relative error for case 1 for k=1

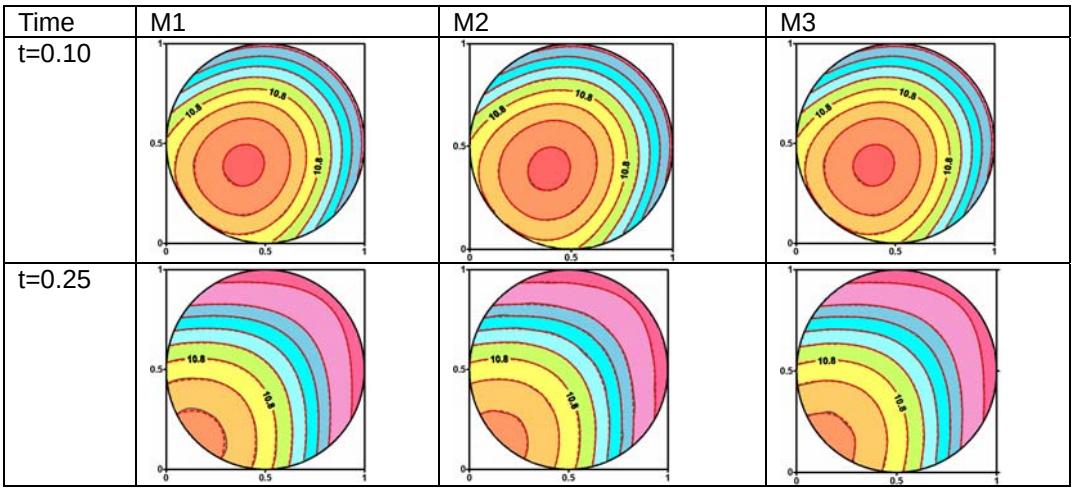


Figure 6: Contour maps of temperature for case 1

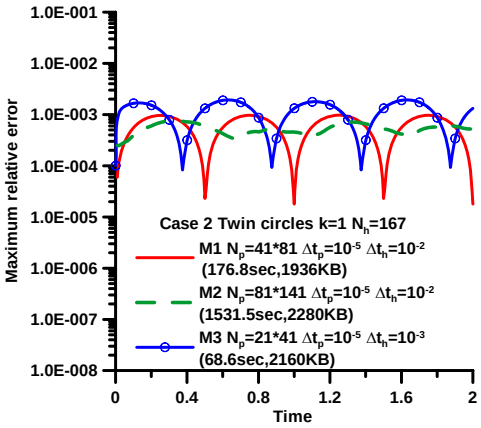


Figure 7: Time history of maximum relative error for case 2

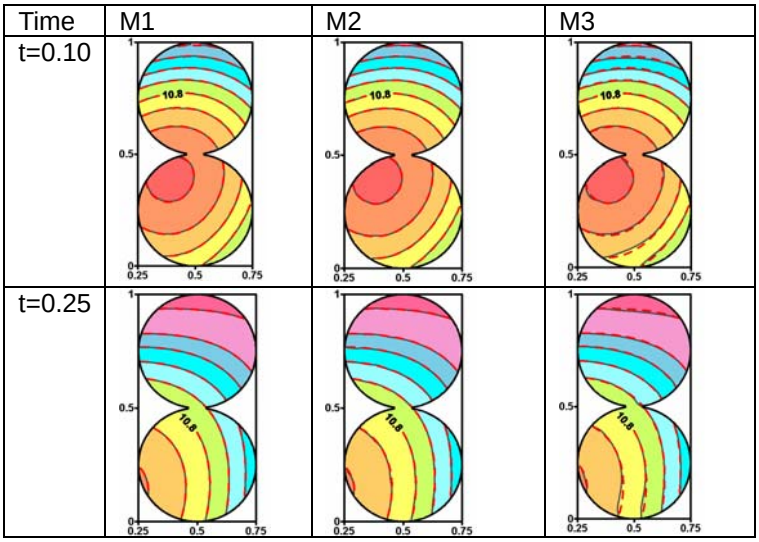


Figure 8: Contour maps of temperature for case 2 using different methods for particular solution